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Crystal structure of bis(4-bromo-2-((3-methylaminopropylimino)-methyl)phenolato)cobalt(II) dinitrate, $[Co(C_{11}H_{15}BrN_2O)_2][NO_3]_2$

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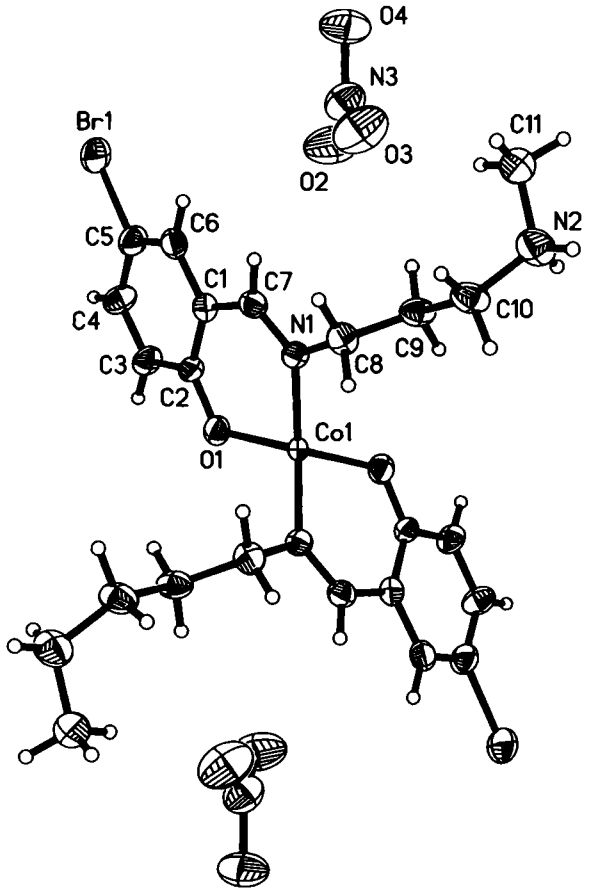

Abstract

$C_{22}H_{30}Br_2CoN_6O_8$, orthorhombic, *Fdd*2 (no. 43), a = 47.639(5) Å, b = 22.047(3) Å, c = 5.451(2) Å, V = 5725.2 Å^3, Z = 8, $R_{gt}(F)$ = 0.053, $wR_{ref}(F^2)$ = 0.126, T = 298 K.

Source of material

Reagents and solvents used were of commercially available quality. 5-Bromo-2-hydroxybenzaldehyde (201.2 mg, 1.0 mmol), *N*-methyl-1,3-diaminopropane (88.3 mg, 1.0 mmol) and $Co(NO_3)_2 \cdot 4H_2O$ (127.5 mg, 0.5 mmol) were dissolved in ethanol (80 ml). The mixture was stirred for 20 min at room temperature to give a clear brown solution. Red block-shaped crystals, suitable for X-ray structure determination were formed by slow evaporation of the solution in dark for a week.

Elemental analysis – found: C, 36.20 %; H, 4.33 %; N, 11.72 %; calc. for $C_{22}H_{30}Br_2CoN_6O_8$: C, 36.43 %; H, 4.17 %; N, 11.59 %.

Discussion

Cobalt complexes of Schiff bases have been extensively studied. They play an important role in both synthetic and structural research [1-3]. In addition, recent investigations have shown that certain cobalt complexes are potent antiviral reagents [4]. As an extension of our work on the structural characterization of Schiff base complexes [5-7], a new mononuclear Schiff base cobalt(II) complex is reported here.

The Co(II) atom located on the inversion center is four-coordinated by two O and two imine N atoms from two Schiff base ligands, forming a tetrahedral environment. The amine N atoms of the pendant propylaminomethyl units are protonated and do not take part in the coordination to the Co atom. The bond lengths and angles subtended at the Co center are typical and comparable to the values observed in other cobalt(II) complexes derived from Schiff bases [8-10]. The title compound crystallizes isostructurally with the analogous Zn compound [11].

Table 1. Data collection and handling.

Crystal:	red block, size 0.27 × 0.28 × 0.32 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	34.45 cm^{-1}
Diffractometer, scan mode:	Siemens P4, ω
$2\theta_{max}$:	55°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	12094, 3243
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2319
$N(param)_{refined}$:	178
Program:	SHELXTL [12]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(2A)	16*b*	0.1428	0.3570	0.6148	0.088
H(2B)	16*b*	0.1385	0.3579	0.8778	0.088
H(3)	16*b*	0.2654	0.1006	–0.2839	0.067
H(4)	16*b*	0.2383	0.0171	–0.3599	0.071
H(6)	16*b*	0.1890	0.0592	0.2006	0.063
H(7)	16*b*	0.1964	0.1411	0.4543	0.055
H(8A)	16*b*	0.2202	0.2608	0.7216	0.061
H(8B)	16*b*	0.1990	0.2065	0.7384	0.061
H(9A)	16*b*	0.1685	0.2559	0.4776	0.066
H(9B)	16*b*	0.1900	0.3095	0.4483	0.066
H(10A)	16*b*	0.1703	0.2797	0.9211	0.076
H(10B)	16*b*	0.1833	0.3417	0.8392	0.076
H(11A)	16*b*	0.1242	0.2629	0.5863	0.144
H(11B)	16*b*	0.1027	0.3095	0.6955	0.144
H(11C)	16*b*	0.1189	0.2650	0.8699	0.144

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Table 3. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Co(1)	8*a*	¼	¼	0.2326(2)	0.0315(5)	0.0265(4)	0.0356(5)	–0.0042(4)	0	0
Br(1)	16*b*	0.18785(2)	–0.03836(3)	–0.1528(2)	0.0852(6)	0.0542(4)	0.1174(7)	–0.0091(4)	–0.0282(5)	–0.0218(5)
O(1)	16*b*	0.25995(8)	0.1800(2)	0.0384(8)	0.055(2)	0.043(2)	0.060(3)	–0.005(2)	0.020(2)	–0.004(2)
O(2)	16*b*	0.1489(2)	0.1548(3)	0.794(1)	0.115(5)	0.126(5)	0.082(5)	–0.046(4)	0.022(4)	0.001(4)
O(3)	16*b*	0.1450(2)	0.1744(3)	1.182(1)	0.134(6)	0.098(4)	0.082(5)	–0.035(4)	–0.033(4)	–0.014(4)
O(4)	16*b*	0.1138(1)	0.1216(3)	0.996(1)	0.070(3)	0.111(4)	0.075(3)	–0.033(3)	–0.002(3)	–0.018(3)
N(1)	16*b*	0.21949(9)	0.2096(2)	0.4182(8)	0.040(3)	0.040(3)	0.037(3)	0.001(2)	0.001(2)	–0.005(2)
N(2)	16*b*	0.1427(1)	0.3336(3)	0.750(1)	0.060(4)	0.089(4)	0.072(4)	0.000(3)	0.014(3)	–0.019(4)
N(3)	16*b*	0.1363(1)	0.1503(3)	0.992(1)	0.082(5)	0.065(4)	0.068(4)	–0.011(3)	–0.012(4)	0.000(4)
C(1)	16*b*	0.2203(1)	0.1200(3)	0.154(1)	0.045(3)	0.040(3)	0.045(3)	–0.006(2)	0.002(3)	0.000(3)
C(2)	16*b*	0.2440(1)	0.1338(2)	0.008(1)	0.042(3)	0.035(3)	0.046(3)	0.002(2)	0.002(3)	0.005(3)
C(3)	16*b*	0.2499(1)	0.0931(3)	–0.184(1)	0.064(4)	0.044(3)	0.060(4)	0.007(3)	0.018(4)	–0.008(3)
C(4)	16*b*	0.2338(1)	0.0429(3)	–0.231(1)	0.074(5)	0.052(4)	0.052(4)	0.015(3)	–0.002(4)	–0.011(3)
C(5)	16*b*	0.2107(2)	0.0311(3)	–0.084(1)	0.063(4)	0.043(3)	0.066(5)	0.001(3)	–0.012(4)	–0.010(3)
C(6)	16*b*	0.2044(1)	0.0682(3)	0.102(1)	0.048(4)	0.048(3)	0.062(4)	–0.009(3)	0.003(3)	–0.006(3)
C(7)	16*b*	0.2106(1)	0.1573(3)	0.358(1)	0.040(3)	0.048(3)	0.049(3)	0.000(3)	0.002(3)	–0.002(3)
C(8)	16*b*	0.2062(1)	0.2379(3)	0.631(1)	0.051(4)	0.057(4)	0.045(3)	–0.003(3)	0.007(3)	–0.011(3)
C(9)	16*b*	0.1831(1)	0.2788(3)	0.561(1)	0.050(4)	0.066(4)	0.050(4)	0.014(3)	–0.003(3)	–0.015(3)
C(10)	16*b*	0.1709(1)	0.3091(3)	0.789(1)	0.047(4)	0.082(5)	0.060(5)	0.010(3)	0.003(3)	–0.022(4)
C(11)	16*b*	0.1202(2)	0.2889(3)	0.723(2)	0.061(5)	0.066(5)	0.160(9)	–0.001(4)	0.009(6)	0.004(6)

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